IMPACT OF MECHANICAL VENTILATION ON BUILD-UP AND CONCENTRATION DISTRIBUTION INSIDE A 1-M^3 ENCLOSURE CONSIDERING HYDROGEN ENERGY APPLICATIONS CONDITIONS OF USE. EXPERIMENTS AND MODELLING

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ABSTRACT

Natural ventilation is an efficient and well-known way to mitigate a hydrogen build-up in the case of an accidental release in confined enclosures. However, for some hydrogen energy applications, natural ventilation is not possible or is not efficient enough to reach defined safety strategy. Thus, mechanical or forced ventilation can be interesting means to avoid critical concentration of hydrogen considering degraded operation and associated potential hazardous events. To better understand the impact of mechanical ventilation on the hydrogen build-up and distribution, a dedicated study was led. First, accidental release scenarios were experimentally simulated with helium in a 1-m^3 enclosure. Several configurations of release and ventilation modes were tested, and are presented in this study. Secondly, analytical and numerical – Computational Fluid Dynamics – calculation approaches were applied and adjusted to propose a simplified methodology, taking into account mechanical ventilation for assessment of hydrogen accumulation and for design optimization of the applications.

1.0 CONTEXT

To avoid hazardous situations in hydrogen applications with confined configurations, one mitigation strategy is to limit hydrogen build-up in case of accidental release. Natural ventilation is a very interesting means of passive mitigation to limit hydrogen accumulation. However in some specific cases (efficiency, design constraints, weather conditions…), natural ventilation cannot bring a satisfying mitigation solution. In these cases mechanical/forced ventilation is a potentially interesting alternative, if well designed and sized.

Actually mechanical ventilation is an efficient way to limit concentration inside a confined enclosure in case of hydrogen release. Compared to natural ventilation, this active mitigation means opens many possibilities in terms of level of ventilation, configuration, location, etc., but understanding and knowledge are required in order to properly design the ventilation system, taking into account the various parameters (such as release flow rate, type of release, internal obstruction, etc) of the accidental scenario to be mitigated.

In this way several approaches were investigated from experimental testing to numerical simulations. Thus, an existing Air Liquide experimental test facility was modified by adding a mechanical ventilation module in order to perform new experiments on hydrogen accumulation in these configurations. The experimental testing apparatus is described below. In parallel numerical simulations were carried out and experiments were adjusted according to the needs of numerical simulations.

In this study, aimed at improving the understanding of the impact of forced ventilation on build-up and concentration distribution, experiments with helium were performed and compared with numerical simulations; numerical parameters were adjusted iteratively in order to establish the most appropriate numerical approach. These results were also compared to existing analytical models.

For safety reasons, helium was used instead of hydrogen for experimental aspects of the study. Helium was already used in previous investigation of buoyant releases to represent the characteristic behaviour of hydrogen, with an associated CFD benchmark [1]. Analogy between helium and hydrogen in terms of dispersion in confined space was demonstrated in a previous work [2].

2.0 DESCRIPTION OF INVESTIGATED APPROACHES

2.1 EXPERIMENTAL SETUP

2.1.1 Description of the test facility

Air Liquide's DRHyS test facility (Dispersion Research for Hydrogen Safety) was used to experimentally assess hydrogen accumulation considering different leak scenarios. The experimental setup consists of an enclosure equipped with a releasing nozzle to simulate different types of leaks inside a confined or a semi-confined enclosure. This test facility enables to study risk scenarios and consequences in terms of build-up and dispersion in case of an accidental leak inside an application using a hydrogen fuel cell technology.

For the safety of the experiments, the DRHyS test bench uses helium as releasing gas instead of hydrogen. Thus the releasing system of the DRHyS test facility is linked to a rack of 200-bar helium cylinders (see Figure 1).

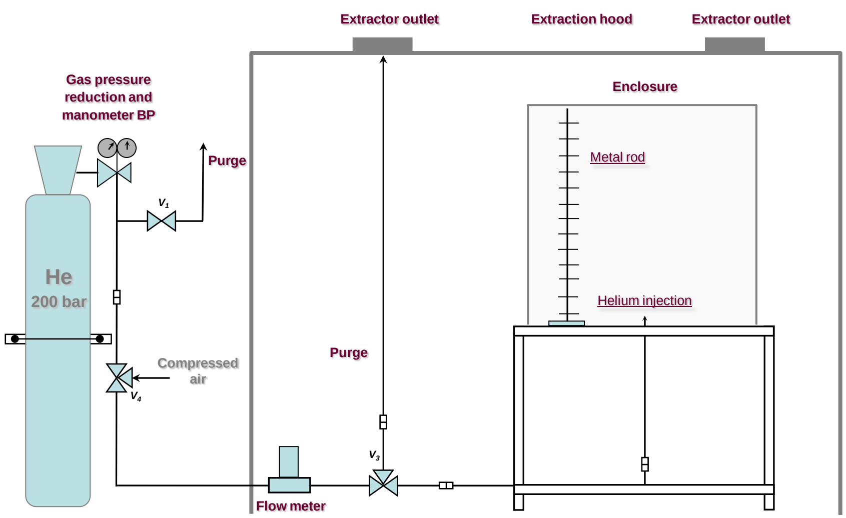


Figure 1. Scheme of the DRHyS test bench.

The experimental enclosure simulating the confinement of the hydrogen application considered is a cube-shaped, polycarbonate enclosure of 1-m^3 internal volume (see Figure 2), with a square base of 0.995 m and a height of 1 m.

Figure 2. The releasing enclosure of the DRyS test bench.

For the present study, the 1-m³ enclosure was connected to a mechanical ventilation system (France Air type MV5/4P) connected at the top of the enclosure to evaluate the effectiveness of the forced ventilation in limiting helium build-up (see Figure 3). The extraction tube had a diameter of 160 mm linked to the mechanical ventilation device with a sheath measuring 3 m long.

Ventilation flow rates were assessed through velocity measured using to an anemometer (AN300 model).

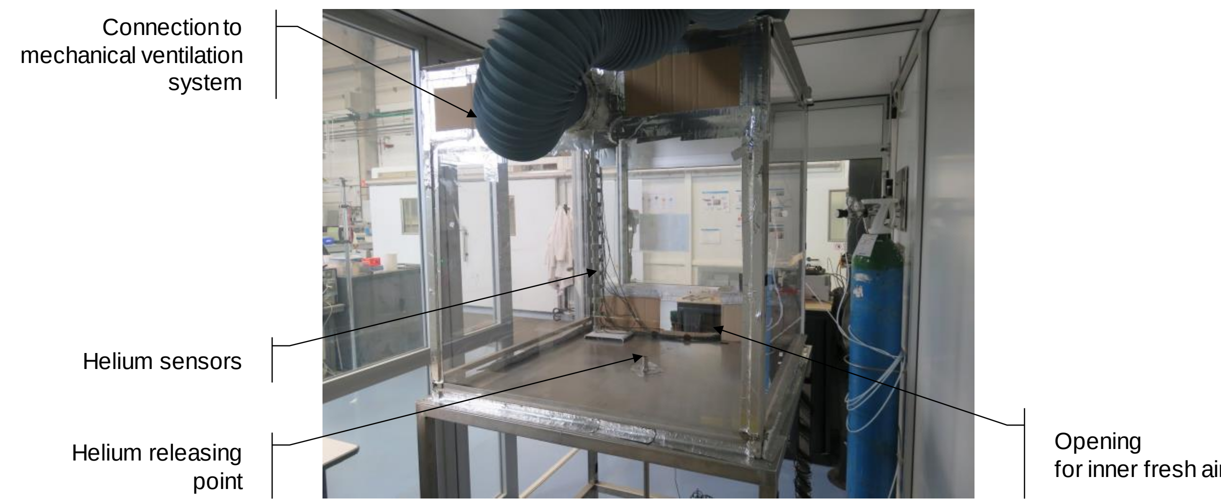


Figure 3. Mechanical ventilation systems.

In this study, the mechanical ventilation was operated in extraction mode; i.e. helium-air mixture is extracted at the top from inside to outside the enclosure.

As shown on Figure 3, a rectangular aperture was placed at the bottom of the enclosure for fresh air entering, on the opposite face of the extraction tube. Sizing - 30-cm length, 15-cm height - was chosen large enough in order to not limite mechanical ventilation extraction flow rate.

2.1.2 Metrological device

Previous results showed that for natural ventilation, the distribution of helium concentration inside the cuboid enclosure was only in one dimension (1D). A specific parametric study was therefore performed in order to determine the most relevant location of the sensors to effectively measure the representative concentrations in forced ventilation configurations. Thus, a metal rod, holding fifteen sensors, was implemented at the opposite end of the extraction aperture, to measure the concentration distribution along the height in the enclosure. The sensors were positioned at constant interval (6.5 cm) from the bottom to the top of the enclosure, as shown in Figure 4.

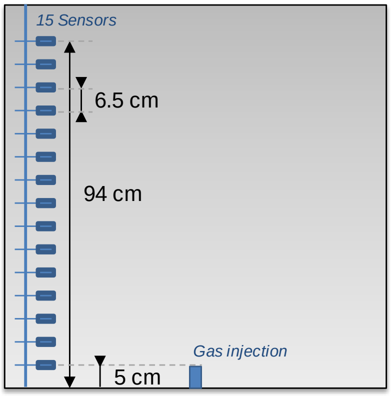


Figure 4. Location of the sensors in the 1-m^3 build-up enclosure.

The sensors used were Xen-TCG 3880 catharometers (also known as thermal conductivity detectors, see Figure 5). Conductivity is measured and helium concentration is directly deduced from this measurement with reactivity (around 1 s) and accuracy (0.02% in absolute). Minicatharometers were specifically calibrated using dedicated helium-air mixtures from 0.5 to 60%-He.

Figure 5. Minicatharometer Xen-TCG 3880.

2.1.3 Experimental procedure

Helium was injected at 5 cm from the bottom of the enclosure – vertically upwards through a circular nozzle of 10-mm internal diameter centered in the horizontal section of the enclosure.

The mechanical ventilation was set at a targeted flow rate. Helium was injected (i.e., released) in the enclosure. The experiment commenced when the targeted flow rate of helium value was reached and correctly regulated by the mass controller. Helium concentrations were measured by the minicatharometers as a function of the time and of the height are recorded each 1 s. The injection was stopped after reaching the steady state; i.e. when helium concentrations were stable in the time.

A previous study showed that final helium concentrations reached at steady state are completely independent of the time of ventilation launching compared to the helium injection time.

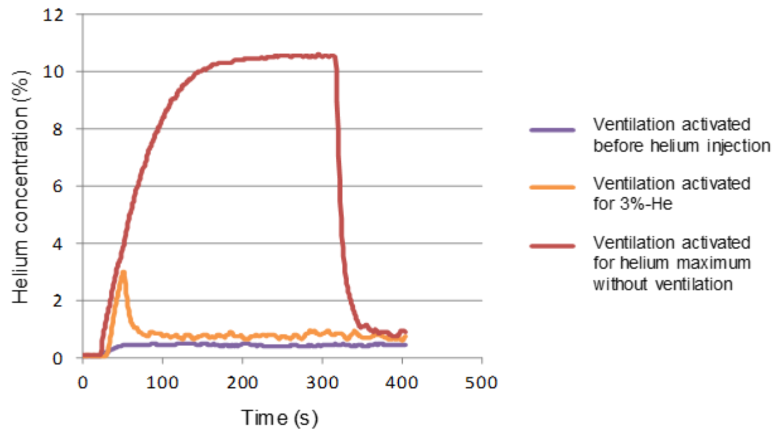


Figure 6. Ventilation activation mode.

During gas injection, the stability of the pressure and of the temperature inside the enclosure was monitored.

2.2 NUMERICAL APPROACH

For CFD modelling a commercial code ANSYS FLUENT 2019 R1 (v193) is used [3]. Fluent is a commercial Fluid Mechanics software which solves Navier-Stokes equations using a finite volume method. In current investigation, a 3-D Cartesian grid is used. Mostly RANS (Reynolds-averaged Navier–Stokes) approach using k-eps and k-omega for turbulence modelling) is applied. LES (large Eddy Simulation) is also performed for one specific case.

In previous studies, RANS simulations [1, 4-5] were compared with experimental data for the dispersion of helium inside closed and semi-confined cubic enclosures. Good agreement was found in these configurations of release and ventilation. The numerical approach used to simulate the forced ventilation and to calculate the distribution of helium concentration in different regimes is presented below.

LES was also used for modelling of helium releases by [6] in a very small enclose of 3.6 10^{-4} m^3 volume.

2.2.1 Meshing strategy

Table 1 shows the meshing characteristics for the numerical simulations. In total, six grids were tested. M1, M2 and M3 are using tetrahedrons for both 2D and 3D meshing. M4, M5 and M6 are using polyhexcore meshing which uses polyhedron for 2D meshing and hexahedrons for 3D meshing. For every mesh, an equivalent mesh for natural convection exist, the unique difference is the geometry which does not include a ventilation tube but a cuboid modelling external air. This cuboid is always existent next to the downer vent.

Table 1. Meshing characteristics.

Mesh	M1	M2	M3	M4	M5	M6
Type of meshing	Tetrahedron	Tetrahedron	Tetrahedron	Polyhexcore	Polyhexcore	Polyhexcore
Number of cells	521k	1M	2.2M	700k	1.5M	2.4M
Edge length [m] (min)	0.001	0.0005	0.0001	0.002	0.0015	0.001
Edge length [m] (max)	0.033	0.029	0.026	0.02	0.015	0.01

For numerical modelling of helium build-up distribution inside a forced ventilated enclosure, M5, a hexahedral mesh of 1.5 M cells was chosen (see Figure 7) as it has been compared with other meshes and gives the best ratio simulation duration / precision.

As an exception, for LES simulation, M6, a hexahedral mesh of 2.4M cells was chosen and has been validated with Pope criterion [7] greater than 85% (80% would have been sufficient) for the volume and Y+ (lower than 5) for near walls treatment.

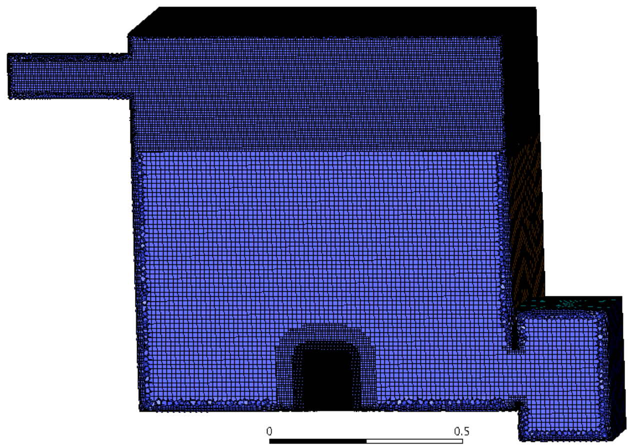


Figure 7. Meshing Hexahedral 1.5 M close to symmetry plane.

2.2.2 Initial conditions

The ambient temperature of air was set to 305.14 K which corresponds to air ambient temperature in the laboratory where the experiments were carried out. The pressure was considered as atmospheric: 101325Pa.

2.2.3 Boundary conditions

The boundaries were divided into four types:

- velocity-inlet (injection and ventilation surface),
- pressure outlet (every surface external which is not an enclosure wall),
- symmetry (see Figure 7),
- and wall (for enclosure walls).

The injection of helium was set to a velocity of 21.22 $m.s^{-1}$; this corresponds to a flow rate of 100 $NL.min^{-1}$.

The ventilation varied from 0 to 300 $m^3.h^{-1}$, which corresponds to a velocity up to 4.145 $m.s^{-1}$.

2.2.4 Viscosity resolution

Three types of viscosity models were tested:

- RANS (Range-Average Navier-Stokes) k-epsilon realizable,
- RANS k-omega SST (Shear Stress Transport),
- and LES (Large-Eddy Simulation)

RANS models do not calculate every eddy, they average them. Historically, “k-epsilon” is supposed to be more efficient far from boundary layer and “k-omega” more efficient in the boundary-layer. The “k-omega SST” model offers good results in both cases. In most industrial cases, it is a common choice as the calculation cost and grid precision dependency is much lower. The LES models offers the possibility to calculate the biggest eddies and still average the smaller ones. The LES calculation cost is a lot more important than RANS but it is more precise, especially in the “direct aspiration regime” (see Figure 11, middle picture) where it has been used.

Finally, k-omega SST viscosity model was chosen to perform numerical calculations.

2.2.5 Temporal and spatial discretization

For spatial discretization, the second order upwind was chosen for momentum, equation k, equation epsilon, equation omega and species equation. Presto! (Pressure Staggering Option) approach is used for pressure velocity coupling.

For time discretization, the second order implicit scheme is used. The CFL is kept moderate (lower than 3.5) during the flow development, then the time step is increased gradually until a steady-state occurs.

2.3 STUDIED CONFIGURATIONS

The experimental and numerical studied configurations are presented in the following Table.

Table 2. Studied configurations.

Parameters	**Values**
Temperature	Ambient temperature, 15°C
Helium flow rate	100 $NL.min^{-1}$
Injection height	5 cm
Internal diameter of the source	10 mm
Bottom opening	h15 x w30 cm*
Top opening	Ø16 cm (circular)
Ventilation flow rate	From 0 to 300 $m^3.h^{-1}$

* *h the height, w the width*

3.0 RESULTS AND DISCUSSION

3.1 EXPERIMENTAL RESULTS

Experiments were performed for several:

- helium injection flow rates,
- injection diameters,
- and ventilation flow rates.

For this study, a focus is done specifically on:

- 10-mm diameter circular injection,
- 100-$NL.min^{-1}$ helium injection flow rates,
- ventilation flow rates up to 300 $m^3.h^{-1}$,
- at steady state; i.e. when helium concentrations are constant.

Figure 8 presents concentration distribution inside the forced ventilated enclosure for several ventilation flow rates.

Q_{v_ref} is the ventilation flow rate reference. Other flow rate magnitude orders are given proportionally to this reference case.

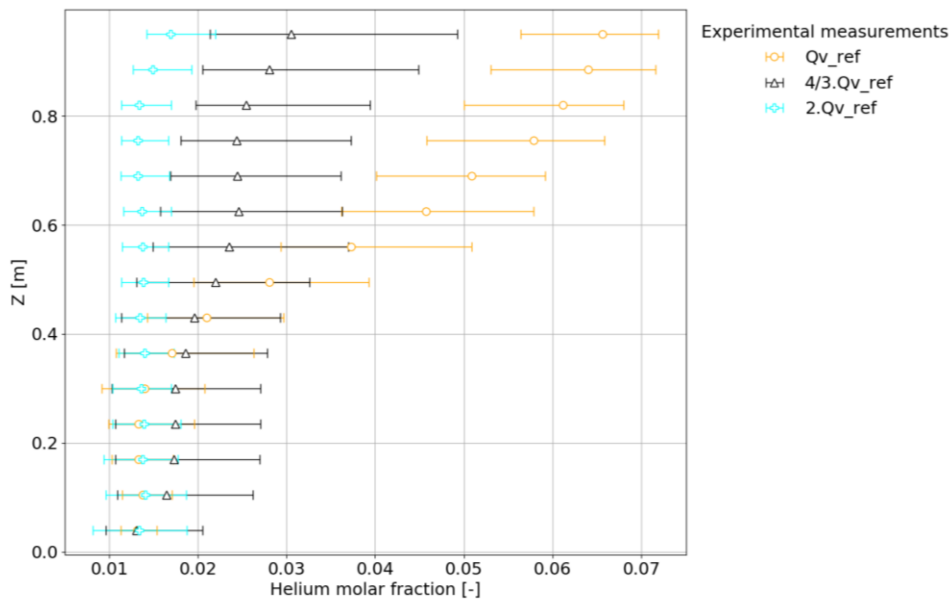


Figure 8. Experimental helium distribution on the height of the 1-m^3 enclosure at steady state according to ventilation flow rate, for 100-NL.min^{-1} helium releasing flow rate.

Data reported on the chart are averaged concentrations calculated on a time slot of 100 s at steady state. Error bars represent experimental fluctuations of measured concentrations (i.e. lower and upper limits).

Figure 8 clearly shows that the ventilation rate has a significant impact on:

- helium concentrations,
- concentration distribution regimes.

Almost three different concentration distribution regimes can be visualized on Figure 8:

- a bi-layered regime for Q_{v_ref},
- a stratified regime for $4/3 \cdot Q_{v\_ref}$,
- a homogeneous regime for $2 \cdot Q_{v\_ref}$.

Actually, the higher the ventilation flow rate, the lower the helium concentrations in the upper part of the enclosure, and the more the distribution regime is far from the bi-layered distribution regime well known for natural ventilation through bottom and top apertures (displacement regime).

For very high level of ventilation, helium concentration becomes homogeneous in the whole enclosure whatever the height.

3.2 NUMERICAL SIMULATION OF MECHANICAL VENTILATION CONFIGURATIONS

3.2.1 Numerical results on helium concentration distribution

Figure 9 presents numerical and experimental helium concentrations obtained at steady state for a helium injection flow rate of 100 $NL.min^{-1}$ and varying forced ventilation flow rates.

Calculated values of helium concentrations - based on RANS numerical approach using a k-omega viscosity model - were compared to experimental data obtained with DRHyS test bench facility.

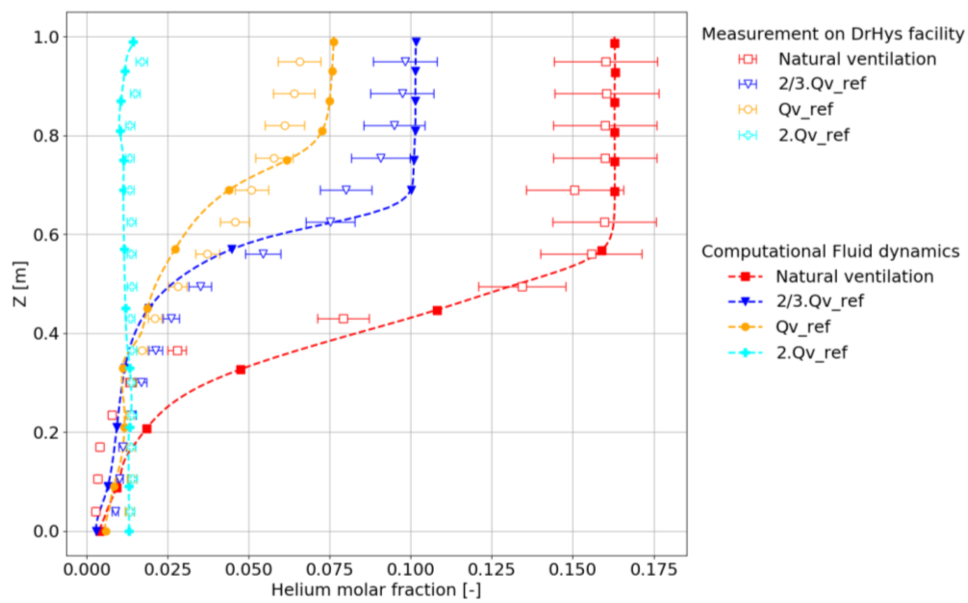


Figure 9. Helium distribution on the height of the 1-m^3 enclosure at steady state according to ventilation flow rate, for 100-$NL.min^{-1}$ helium releasing flow rate. Numerical and experimental data.

Data reported on the chart are averaged concentrations calculated on a time slot of 100 s at steady state. Error bars represent concentration relative deviation of ± 10%.

Figure 9 shows a satisfying agreement between determined numerical approach and experimental measurements.

Calculated concentrations are very close to experiments, at least in the upper and lower parts of the enclosure. The most significant deviations are observed in transition areas:

- for some heights in the enclosure,
- for ventilation flow rates corresponding to “intermediate” distribution regimes.

Figure 10 gives a focus on maximal concentrations obtained experimentally, numerically (with LES end k-omega approaches) and analytically with a simple approach.

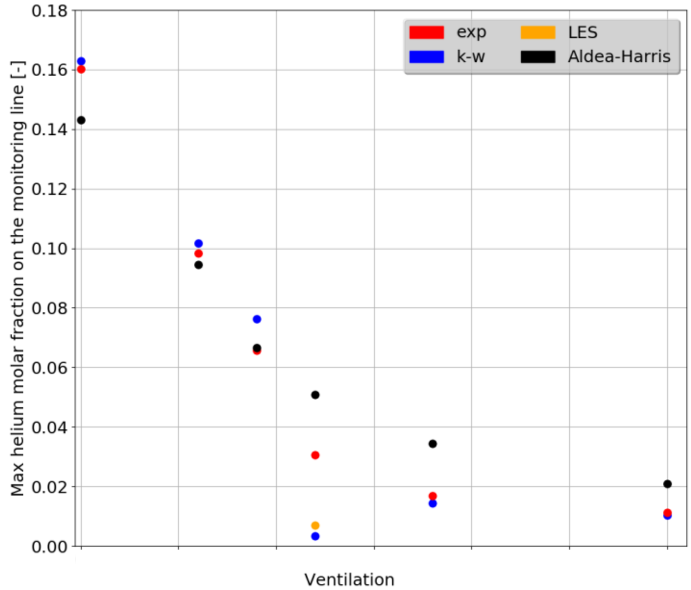


Figure 10. Experimental, numerical and analytical helium maximal concentration at steady state for 100-NL.min^{-1} helium releasing flow rate according to ventilation flow rate.

Except for a specific forced ventilation flow rate, a good agreement is observed between calculated values and experimental measurements. A complex transition phase is believed to exist for the critical ventilation value where deviations are significant. More investigations are in progress around this forced ventilation magnitude order. For this specific case, a LES numerical approach was tested, but the results were not improved.

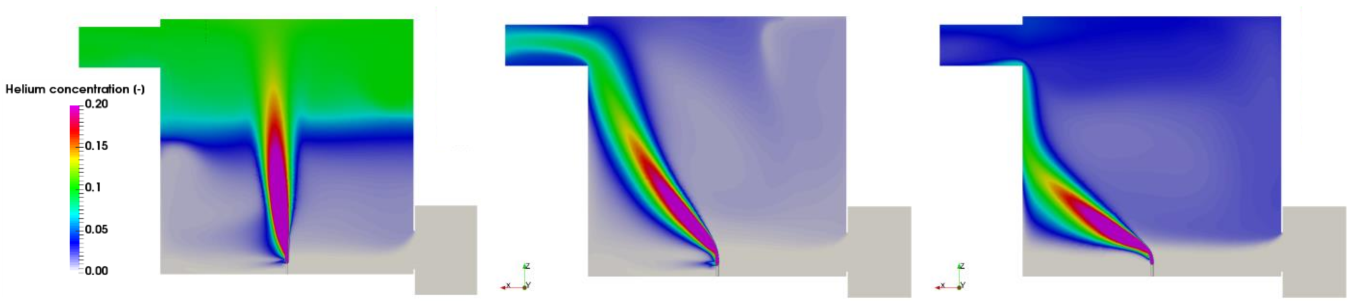
For high ventilation levels, the ALDEA-Harris analytical approach [8] overestimates helium concentrations. Thus, other analytical approaches have not yet been tested. Results obtained experimentally and numerically will be used to improve these kind of approaches, which are very useful for developing simple and quick calculation tools.

3.2.2 Numerical focus on ventilation impact on helium jet

Figure 11 shows the impact of forced ventilation on helium jet.

As the ventilation flow rate is increased, the impact on the helium jet is more important. For the highest values of ventilation flow rate, the helium jet is significantly bent.

For some cases, it is likely that the jet is directly oriented in the outlet flow, induced by the ventilation, without mixing with the other parts of the enclosure (see Figure 11, middle picture); far from the helium jet, concentrations should be very low. This behaviour could explain discrepancies observed between calculated concentration values and experimental measurements previously highlighted. More analyses are in progress.



$2/3 \cdot Q_{v\_ref}$ $4/3 \cdot Q_{v\_ref}$ $2 \cdot Q_{v\_ref}$

Figure 11. Mechanical ventilation impact on helium jet.

4.0 CONCLUSIONS

Forced ventilation was studied through several approaches in order to better understand impact of this active mitigation method on helium accumulation inside an enclosure for risk management and safety of specific hydrogen energy applications.

Experimental measurements were performed - with helium for safety reasons - and numerical approaches were tested and compared to experiments in order to define an efficient and accurate approach.

A satisfying CFD approach was described and validated using a k-omega viscosity model.

Calculated maximal helium concentrations are in good agreement with experiments and concentration distribution regimes are well defined.

However a strange and complex behaviour was highlighted for intermediate ventilation flow rates which certainly correspond to a phase transition. Some actions are in progress in order to better understand this critical field.

In parallel, analytical approaches are investigated in order to develop simple, quick and accurate calculation tool for non-expert users, using knowledge built through experimental and numerical works presented in this study.

In the very last stage of this development, it will be required to adapt approaches to hydrogen, but existing studies have already demonstrated this feasibility [2].

Additionally, it is planned to extend this study to larger volumes, close to iso-containers dimensions.

ACKNOWLEDGMENTS

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